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G parity boundary conditions and $\Delta I = 1/2$, $K \to \pi\pi$ decays

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The use of G-parity boundary conditions to compute $\Delta I = 1/2$, $K \to \pi\pi$ decays is reviewed and a method to consistently treat both the pions and kaon in full QCD proposed. This approach creates a physical, final-state, pion momentum using a 3 fm box and avoids statistical noise coming from pions with smaller momentum.

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The violation of CP symmetry in the two pion decays of the K meson offers an important opportunity to uncover new sources of CP violation beyond those predicted by the standard model. Of special interest is the direct CP violation parameterized by ε' which is now experimentally determined on the 10% level and sensitive to possible new phenomena on the TeV scale. An accurate calculation of this quantity within the standard model requires the evaluation of matrix elements of four-Fermi operators between K and $\pi - \pi$ states. Such matrix elements are within the reach of lattice QCD methods. However, the presence of two particles in one of the states and the need to the evaluate "vacuum" or "disconnected" diagrams, in which the initial and final states are joined only by the exchange of gluons, make these calculations particularly difficult.

Here we focus on the difficulties of the $\pi - \pi$ final state, especially the $I = 0$ state with vacuum quantum numbers. An attractive approach to these two-pion states uses chiral perturbation theory to relate the two pion matrix elements of interest to simpler matrix elements between the K meson and a single pion or the vacuum state. Unfortunately, recent results [1, 2] suggests that $SU(3) \times SU(3)$ chiral perturbation theory works poorly at the kaon energy leading to large systematic errors from this approach. Thus, calculation of actual $\pi - \pi$ matrix elements have become important.

1. Overview of finite volume methods

The methods of lattice QCD construct the eigenstates of the full QCD Hamiltonian $H_{\rm QCD}$ by studying Green's function of interpolating operators at large separations in Euclidean time. In this way the contribution of that eigenstate with the lowest eigenvalue of $H_{\rm QCD}$ is exponentially enhanced. This results in the difficulty of Maiana and Testa [3] that when studying $K \to \pi\pi$ decays the energy non-conserving matrix elements with the state of two pions at rest will be computed.

As is now well understood, this difficult can be diminished by exploiting the finite volume in which lattice calculations are necessarily performed. In finite volume the $\pi - \pi$ eigenstates of $H_{\rm QCD}$ are a series of discrete states with energies shifted in a known way from those of two free particles in a box by the $\pi - \pi$ interaction [4, 5].

However, working in finite volume also introduces a difficulty. The finite volume eigenstates of $H_{\rm QCD}$ are necessarily mixtures of different angular momenta because the usual cubic box is asymmetric under rotations. Thus, the matrix element of a local weak operator Q_i between the K meson and finite-volume $\pi - \pi$ eigenstate, $\langle K|Q_i|\pi\pi\rangle$, is a product of the desired $l = 0$ decay amplitude and the amplitude for finding this $l = 0$ state within the normalized finite volume $\pi - \pi$ eigenstate which is a superposition of different values of l. This problem has been solved by Lellouch and Luscher [6]. The needed correction can be made to adequate accuracy once the $\pi - \pi$, $l = 0$ scattering phase shift has been determined for the relevant isospin chanel and energies.

Three methods that have been developed to deal with these finite volume states. In the first, one tunes the linear size L of an $L^3 \times T$ space-time volume so the $2\pi/L$ (or more accurately the quantized momentum which is determined by the $\pi - \pi$ scattering phase shift $\delta(I)_{l=0}$) so that the first excited $\pi - \pi$ state has the energy of the kaon. For a physical pion this requires $L = 6$ fm. While appealingly simple, in this approach the state of interest, $|\pi\pi(p \approx 2\pi/L\rangle$, is in fact the third lowest energy state that will contribute to the Green's function being computed: both the vacuum (for $I = 0$ and the $p \approx 0$ $\pi - \pi$ state will have lower energy. Extracting the decay matrix element from such a three-exponential description of this Green's function time dependence will be difficult.

A second method, which results in the $\pi - \pi$ state possessing the lowest energy of all allowed states, gives the initial kaon a non-zero 3-momentum. The two final pions must also carry this momentum. The lowest energy $\pi - \pi$ state with $\vec{p} \neq 0$ will contain one pion which is nearly at rest and a second which carries the kaon momentum. An energy conserving decay will result if the kaon and one final pion carry 740 MeV of momentum. For a 3.5 fm box (too small to avoid large finite volume corrections at the physical pion mass) the kaon and pion momenta would need to be $\approx 2 \cdot 2\pi/L$. Such large momentum amplitudes are expected to be noisy and difficult to compute.

This approach with a non-zero center (cm) of mass momentum has been explored theoretically [7, 8] and a first calculation shows encouraging results [9]. Since the vacuum cannot carry momentum, the lowest energy state which contributes to such non-zero cm momentum correlators will be the $\pi - \pi$ state of interest, even for $I = 0$. This approach deserves further study.

A third approach, which is the topic of the remainder of this article, is the use of boundary conditions to eliminate the $p \approx 0$, $\pi - \pi$ state. There are two techniques of interest. The first, which can be applied to only the $I = 2$, $\pi - \pi$ state, imposes anti-periodic boundary conditions on one of the two flavors of light quarks making up the pions. This use of twisted boundary conditions with a twist angle $\theta = \pi$ was introduced in Ref. [10] where they were called H-parity boundary conditions. For the case of $\Delta I = 3/2$ decay, the $\pi - \pi$ final state will have $I = 2$ and isospin symmetry can be used to relate the matrix element of interest to a matrix element involving the $|\pi^+\pi^+\rangle$ state. With H-parity boundary conditions, the π^+ meson will obey anti-periodic boundary conditions forcing the pions in a $\pi^+ - \pi^+$ state with zero cm mass momentum to have a relative momentum of $\pm\pi/L$ in the direction orthogonal to the 2-d face on which the boundary conditions are applied. Since this $\pi^+ - \pi^+$ state is the unique $\pi - \pi$ state with charge 2, the use of isospin breaking boundary conditions does not lead to unwanted mixing of the $I = 0$ and $I = 2$ final states. Finally because all $\pi - \pi$ intermediate states must contain the valence quarks on which the boundary conditions have been imposed, such H-parity boundary conditions can be imposed on only the valence quarks, using a lattice ensemble generated with normal boundary conditions [11]. This is an attractive method to compute the $\Delta I = 3/2$ kaon decay amplitude [12, 13].

A second type of boundary condition which can be imposed to insure that the final-state pions carry non-zero momentum is G-parity boundary conditions [14]. Since all three pions are odd under G-parity, these boundary conditions imply that each pion must have $p_i \approx \pm\pi/L$ when these boundary conditions are imposed on the face perpendicular to the i^{th} direction. We now discuss these boundary conditions in more detail.

2. G-parity boundary conditions for the pions

Recall that the G-parity transformation composes the charge conjugation operator with an isospin rotation about the *y*-direction. This transformation commutes with the three generators of isospin and changes the sign of an iso-triplet whose third component, in our case the π^0, is charge conjugation even. On the level of the quark fields creating u and d quarks, $(\overline{u}, \overline{d})$ G-parity has the following action:

$$G \begin{pmatrix} \overline{u} \\ \overline{d} \end{pmatrix} G^{-1} = \begin{pmatrix} C d^{\mathrm{T}} \\ -C u^{\mathrm{T}} \end{pmatrix} \tag{2.1}$$

where C is the 4×4 charge conjugation matrix which obeys $C\gamma^\mu C^{-1} = -(\gamma^\mu)^{\mathrm{T}}$. Here and in Eq. 2.1 above, the superscript T indicates the transpose of a 4×4 and a 1×4 matrix respectively. Such G-parity boundary conditions are ideal for our problem, respecting isospin symmetry while yielding a lowest energy state of the two pions of the form:

$$E_{\pi\pi} \approx \sqrt{n\left(\frac{\pi}{L}\right)^2 + m_\pi^2}. \tag{2.2}$$

where $n = 0$, 1, 2, 3 is the number of spatial boundaries on which the G-parity condition is imposed. The appearance of π/L rather than $2\pi/L$ means that smaller energies are accessible.

Two difficulties must be overcome when implementing these boundary conditions. First the gauge links that cross a boundary across which G-parity is imposed connect quark fields that transform as SU(3) color triplets and anti-triplets. Thus, these links must transform under a gauge transformation V(x) as $U_\mu(x) \to V(x)U_\mu(x)V(x+(1-L)\hat{e}_\mu)^{\mathrm{T}}$ assuming that the site x is adjacent to a boundary which the link $U_\mu(x)$ crosses and that L is the lattice size in the μ direction. This modified transformation law requires a modified gauge action for all plaquettes which straddle this boundary. For x and μ as above and $\nu \neq \mu$ we must use $\mathrm{tr}\big(U_\mu(x)U_\nu(x+(1-L)\hat{e}_\mu)^* U_\mu(x+\hat{e}_\nu)^{-1}U_\nu(x)^{-1}\big)$. Of course, the required change in the gauge action can be made and the resulting theory will still be translationally invariant provided the translation operation is generalized to include replacing some gauge links with their complex conjugate. This altered gauge action requires that a new ensemble of gauge field be generated for each assignment of G-parity boundary conditions.

The second complexity is the presence of charge conjugation in the definition of G-parity. Typically a Dirac operator that includes such a charge conjugation will be represented by a path integral which evaluates to Pfaffian [15] rather than a more familiar determinant. However, for our two-flavor case there is no direct coupling between a Grassmann integration variable and itself. For example, u couples to $\overline{d}$ which then couples to $-u$ as one traverses the lattice twice in a direction perpendicular to a face across which G-parity conditions are imposed. Thus, we can view the u quark as a Grassmann variable defined on a doubled volume where the u degree of freedom on the extention of the original volume actually equals $\overline{d}$. The result is a standard theory of a single flavor of quark obeying anti-periodic boundary conditions on a doubled lattice volume. While this prevents the second quark from being represented by a simple change of an N_f factor appearing in the evolution algorithm from 1 to 2, the only real cost is a factor of two in the lattice volume that must be studied. This added factor of two cost remains as G-parity is imposed in additional directions. However, the resulting geometry becomes more complex than an $L \times L \times 2L$ three-volume with simple boundary conditions relating the values of the Grassmann u variable on opposite faces.

Thus, G-parity boundary conditions can be imposed on the u and d quarks with no difficulty beyond the doubled space-time volume. Initial numerical simulations have uncovered no serious problems beyond enhanced finite-volume effects that come from the possible binding of an isolated quark to its own, distant, charge-conjugate image.

3. G-parity boundary conditions for the kaon

However, we must now decide how to treat the strange quark. The imposition of charge conjugation boundary conditions on the gauge field implies that the strange quark cannot obey

standard periodic or anti-periodic boundary conditions. There are two natural options to consider. The strange quark could obey charge-conjugate boundary conditions. Alternatively the strange quark could be made part of an artificial pair of degenerate quarks which transform as an isospin doublet and obey G-parity boundary conditions. We consider each of these possibilities in turn.

Let us first impose C boundary conditions on a single species of strange quark. Begin with the standard Grassmann action for the strange quark and then rewrite one half of that action by reversing the order of the s and $\overline{s}$ fields:

$$\overline{s}\not{D}s = \frac{1}{2}\begin{pmatrix} s^{\mathrm{T}} & \overline{s}\end{pmatrix}\cdot\begin{pmatrix} 0 & -\not{D}^{\mathrm{T}} \\ \not{D} & 0\end{pmatrix}\cdot\begin{pmatrix} s \\ \overline{s}^{\mathrm{T}}\end{pmatrix} = \frac{1}{2}\Psi^{\mathrm{T}}\cdot\begin{pmatrix} 0 & -\not{D}^{\mathrm{T}} \\ \not{D} & 0\end{pmatrix}\cdot\Psi \quad \text{where} \quad \Psi = \begin{pmatrix} s \\ \overline{s}^{\mathrm{T}}\end{pmatrix}. \tag{3.1}$$

The standard boundary conditions appear as off-diagonal terms in the Dirac operator $\not{D}$. We can change these boundary conditions to charge conjugation boundary condition by removing this off-diagonal term from $\not{D}$ and putting it into the diagonal blocks labeled as zero in Eq. 3.1. If the Dirac operator without this diagonal term is written as $\not{D}'$ this change in boundary conditions will result in a new action which can be written schematically as:

$$\Psi^{\mathrm{T}}\cdot\begin{pmatrix} \begin{bmatrix} 0 & \Delta \\ -\Delta^{\mathrm{T}} & 0\end{bmatrix} & -\not{D}'^{\mathrm{T}} \\ \not{D}' & \begin{bmatrix} 0 & \Delta' \\ -\Delta'^{\mathrm{T}} & 0\end{bmatrix}\end{pmatrix}\cdot\Psi \quad \to \quad \overline{\Theta}\cdot\begin{pmatrix} \begin{bmatrix} 0 & \Delta \\ -\Delta^{\mathrm{T}} & 0\end{bmatrix} & -\not{D}'^{\mathrm{T}} \\ \not{D}' & \begin{bmatrix} 0 & \Delta' \\ -\Delta'^{\mathrm{T}} & 0\end{bmatrix}\end{pmatrix}\cdot\Theta. \tag{3.2}$$

where the off-diagonal term Δ implements the coupling of $s(x,y,z=L-1,t)$ and $s^{\mathrm{T}}(x,y,z=0,t)$ for the case of charge conjugate boundary conditions in the z-direction and a lattice with L sites in that direction. Similarly Δ' connects $\overline{s}^{\mathrm{T}}(x,y,z=L-1,t)$ and $\overline{s}(x,y,z=0,t)$.

The operator on the left side of the expression 3.2 is the desired Dirac operator with charge conjugation boundary conditions. Grassmann integrals with this action and the integrand $\Psi(x)\Psi(y)^{\mathrm{T}}$ will give the inverse of the Dirac operator obeying these boundary conditions times the Pfaffian of that operator. A practical way to evaluate that Pfaffian is indicated by the term on the right of Eq. 3.2 where the number of independent fermion fields has been doubled so that the single field Ψ has been replaced by two fields Θ and $\overline{\Theta}$. This second action is entirely standard and would yield a normal determinant, the square of the Pfaffian of interest. The resulting Dirac operator is defined in a volume doubled in the z-direction and obeying periodic boundary conditions in that doubled direction. Using the usual rational hybrid Monte Carlo method, we could easily perform a dynamical simulation using the square root of this usual determinant and recover the desired Pfaffian. If domain wall fermions are used with non-zero fermion mass, this determinant is guaranteed to be positive so its square root is well defined. Given the connectivity of the gauge field integration volume, we can then choose a consistent sign for this square root which will be valid throughout that integration volume.

While it is encouraging that charge conjugation boundary conditions are practical to implement, they will not solve our problem. For example, a K^0 meson, created from these strange and light quarks, which is an eigenstate under translation by L in the z-direction will have the from $(\overline{s}d \pm is\overline{u})/\sqrt{2}$ where, from the perspective of the doubled lattice volume in the z-direction, the left-hand term describes the particle for $0 \le z < L$ and the right-hand term applies when $L \le z < 2L$.

Unfortunately, under this translation by L, these states have eigenvalue $\pm i$ and therefore carry momentum $\pm\pi/2L$ so that a momentum conserving 2 pion decay is not possible. This should be expected since $s(x)$ is even when translated in the z-direction by $2L$ while the light quark field is odd, implying that the K meson will satisfy anti-periodic boundary conditions in this expanded $2L$ volume and carry momentum $\pm\pi/2L$.

Note that the odd mixture of particles making up the K meson does not create a problem. By using a weak operator with the correct particle content, we can insure that only the physical $\bar{s}d$ part of the initial state will contribute. The effect of the unusual mixture in this initial state is only on its normalization, introducing a factor of $1/\sqrt{2}$ which can be easily be removed. In the doubled-volume language, such a physically correct choice for the weak operator must involve fields in only one half of the doubled volume which are therefore not translationally invariant so that conservation of momentum must be imposed by the (here impossible) choice of initial and final states.

The second alternative of introducing a fictitious iso-doublet which is made up of the strange quark and a second "charm" quark, (c,s) avoids the non-zero momentum problem discovered above. Now both quarks in a generalized initial kaon state will change sign under translation through $2L$ so a state with zero momentum becomes possible. The ground state which contains the desired $\bar{s}d$ component will be

$$|K^0\rangle = \frac{1}{\sqrt{2}}\,(\bar{s}d + c\bar{u})\,. \tag{3.3}$$

This state is translationally invariant and consistent with the boundary conditions permitting it to carry zero momentum as required.

With this choice of boundary conditions for the strange quark we have effectively doubled the number of flavors in the strange quark sector. Directly using the determinant of this doubled Dirac operator as the weight in the QCD path integral would be incorrect because QCD has one not two flavors of strange quark. Apparently the best solution to this problem is to use the square root of this determinant. This square root will correspond to the correct number of flavors but will add non-locality since such a square root cannot be realized by a local Grassmann path integral. Of course, in contrast with the rooting used with staggered fermions, any effects of this non-locality will disappear in the limit of large volume. The Dirac operator in question differs from the doubled Dirac operator obeying charge conjugation boundary conditions on the right side of Eq. 3.2 by boundary terms and the determinant of this doubled operator obeying charge conjugation boundary conditions is the square of a positive Pfaffian which is appropriately local.

One might also worry that taking such a square root introduces a miss-match between the treatment of the valence and sea quarks. Again such non-unitary effects are expected to be exponentially suppressed for the case of single-particle states such as our K meson in which there is no mixing between the valence and sea quarks [11].[1]

[1] It is interesting to note that this situation is very similar to the use of a superposition of propagators obeying periodic and anti-periodic boundary conditions in the time direction, often done to reduce finite volume effects. The eigenvectors of the Dirac operator defined on the doubled lattice divide into states either periodic and anti-periodic under translation through the original time extent T. Thus, the determinant of the Dirac operator defined on the doubled lattice is the product of the determinants of the Dirac operators defined on the original lattice obeying periodic and anti-periodic boundary conditions. Using the correct number of flavors would require taking the square root of this determinant which is then also not quite a perfect square.

4. Conclusions

The use of G-parity boundary conditions for the up and down quarks and for an iso-doublet made of degenerate strange and fictitious charm quarks allows an accurate description of $K \to \pi\pi$ decays in which the finte-volume energy of the two-pion final state is quantized and the unphysical state with approximately zero relative momentum forbidden. This approach is computationally demanding, requiring a new set of gauge configurations for each choice of boundary conditions. However, for a computationally difficult problem such as posed by the $\pi - \pi$ state with $I = 0$, the generation of the gauge configurations may not be the dominant cost and this approach may yield better-controlled errors than the competing method of using a 740 MeV center of mass momentum.

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